To: technicalreports@afosr.mil
Subject: Final Report to Dr. Michael Berman

Contract/Grant Title: Molecules and Their Interactions: The Development of New Theory and Its Implementation

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Accomplishments:

A. The Relationship Between Fock-Space Multi-reference CC and EOM-CC:
This year much effort was devoted to detailing the relationships between two different methods of treating excited states in CC theory **[9,12, 14, 17,18]**. Today the EOM-CC approach is well-established, after being introduced by us in the 90's. It is widely used for many problems like the treatment of electronic (UV-vis) and photoelectronic spectra. Even more significantly, it is quite valuable as a 'target state method', meaning the state of interest can be better described via the EOM-CC framework than it can be within the usual single-reference CC approach. An example is the treatment of open-shell singlet states that are formally exact in the operationally single-reference CC approach (ie no decisions except choice of basis and level of correlation), but would otherwise require the use of two determinants (or a multi-reference description) in a more conventional approach. This occurs because EOM-CC diagonalizes a matrix that would have both, equivalent determinants in it, allowing them to be weighted however warranted. The same is true for more complicated low-spin cases. Even more complicated multi-reference character can be introduced by using the flexibility inherent in EOM-CC to start from a problem with a different number of electrons to correctly describe a problem, as in using O_3^{-2} to obtain a description of O_3, by removing two electrons from the anion to correctly describe the quasi-degeneracy between the two homo orbitals in ozone.

The alternative FS approach uses a multi-reference description to accomplish some of the same things, but has the advantage over EOM-CCSD, eg, in that that method would require the diagonalization of a matrix of the dimension of all single and doubleexcitations, while the FS approach would get its answers from only the diagonalization of a matrix of the dimension of singles alone, which are much fewer. Furthermore, the FS approach formally derives from an exponential ansatz for the excited states, while the EOM-CC excited states, contrary to the ground state, use a linear (CI-like) operator. The numerical distinction is modest, but can be observed in the limit where an excited state would separate into A+ and B-. We refer to this as 'charge-transfer' separability. All other excited states would go to A* + B* in either method.

Hence, in an attempt to get the best of both worlds, we have embarked upon the detailed relationship between the two methods. This has been accomplished by

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13. SUPPLEMENTARY NOTES

14. ABSTRACT

Accomplishments made during this reporting period include the further development of multi-reference Fock space coupled-cluster theory, with emphasis on its relationship to the equation-of-motion CC method for excited states. The importance of these studies is that each approach has some advantages and disadvantages. The hope is to combine them into one method with the best of both. In addition this period includes our introduction of the new nCC hierarchy which means it has to be exact for n electrons, but is computationally simpler than the corresponding traditional CCSD, CCSDT, CCSDTQ, etc. hierarchy. The seamless connection between correlated wavefunction theory and the effective, one-particle density functional theory which leads to ab initio density dft has been further developed. Also discussed is further work on the massively parallel ACES III program system.

15. SUBJECT TERMS

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invoking the Intermediate Hamiltonian approach in FS-CC, and relating it through the Bloch equation to EOM-CC. Because of the formal relationships we have established, we now have a route toward treating any sector of FS, ie any number of electrons outside a closed shell, which had previously proved to be almost impossible beyond the 1 hole 1 particle sector; by straight-forward matrix diagonalization, a very stable procedure. Also, EOM-CC has always provided a route toward treating properties, but FS-CC has not. Exploiting the inter-relationships, we now can overcome this limitation of the FS-CC approach and gain from its simpler computational aspect and superior formal aspects.

In the course of doing this, we also presented the first results for FS-CCSDT[14], and, in particular, for the FS-CCSDT for triplet states[17,18]. We also investigated the route to low-spin states in EOM-CC via the spin-flip idea of Krylov, meaning use the high-spin triplet or higher as a reference and flip the unpaired spins to get an approximation to a low-spin eigenstate via the EOM-CC approach[12, 23]. This further enhances what states can be described within EOM-CC with minimal decisions for the user.

B. A New Hierarchy for CC theory:

 In last year's report, we focused on this development. Briefly, in the nCC Heirarchy[2], we insist that the method be exact for 2, nCCSD, 3, nCCSDT, and 4, nCCSDTQ electrons. Hence,

E(CISD)=E(CCSD)=E(nCCSD) for n=2;
E(CISDT)=E(CCSDT)=E(nCCSDT) for 3,
E(CISDTQ)=E(CCSDTQ)=E(nCCSDTQ) for 4.

All nCC methods are also extensive. Hence, whereas when we obtain the energy from CI we have the well-known size-extensivity failure, E[CISD(A+B)]≠ECISD(A)+ECISD(B) when A and B are non-interacting two electron units, it follows that

E[CISDTQ] = E[CCSDTQ]=E[nCCSDTQ]
   = E[CCSD(A)]+E[CCSD(B)]
            = E[nCCSD(A)]+E[nCCSD(B)]

That is, all products of non-interacting two-electron units are exact in nCCSD. Similarly, all products of 2, 3 and 4 electrons also give the exact energy for all their combinations. Hence, nCC enables us to think about electron correlation in conceptually appealing 2, 3, and 4 electron units. This also facilitates our understanding of bond breaking, as such units will occur as the separated products after a bond fission. If we can ensure a smooth transition to the products by CC, then we will have a route toward improving the bond breaking in any single reference (UHF, RHF, or other like Brueckner or a KSDFT reference.

Because of nCCSD being exact for two electrons, and all products of two electrons, it is the natural zeroth-order approximation for the separated electron pair bonds in chemistry, which we are further studying in our Natrual Linear Scaling CC approach (NLSCC)[10,11] . Furthermore, the transition from CCSD to nCCSD eliminates the most time-consuming steps in the evaluation of the non-linear terms in CCSD. The normal scaling of such terms is $\sim N^3$ with the number virtual orbitals. However, they can be eliminated leaving just the non-linear terms that scale as $\sim N^2$.Nonetheless, the method is exact for two electrons, and all products of two electrons as it is still composed solely of linked diagrams as required by its extensivity. Furthermore, it still retains all the invariance properties of CCSD, meaning that it is invariant to transformations among just occupied or virtual orbitals. This distinguishes this method from CEPA-like approximations that are not invariant to orbital rotations. Finally, nCCSD has the same orbital insensitivity as does CCSD, since the $\exp(T_1)$ operator is not truncated. The nCC approach coupled-with NLSCC is being implemented into ACES III, the completely newly written, massively parallel version of ACES II. In this way very large molecules will be studied.

C. ACES III and massively parallel implementations.

From scratch, we have written ACES III over the last few years **[15, 20]** and are now starting to reap the benefits. As shown below, we have achieved virtually perfect scaling to 1024 processors and even 85% scaling up to 4096. We have also successfully run on >30000 processors. What this means is that soon it will be almost routine to make CC applications on 10,000 processors, which is normally considered the terascale, with the petascale in prospect. Furthermore, since ACES III provides CCSD and CCSD(T), for open and closed shells, with any single determinant reference function, and analytical gradients for same, [plus EOM-CC for excited states, [lus its IP- and EA-EOM variants, it can be used in plethora of applications to provide 'benchmark' accuracy that were previously thought to be well beyond the reach of CC theory. This development will offer a paradigm change in the field.

CCSD scaling results for various molecules
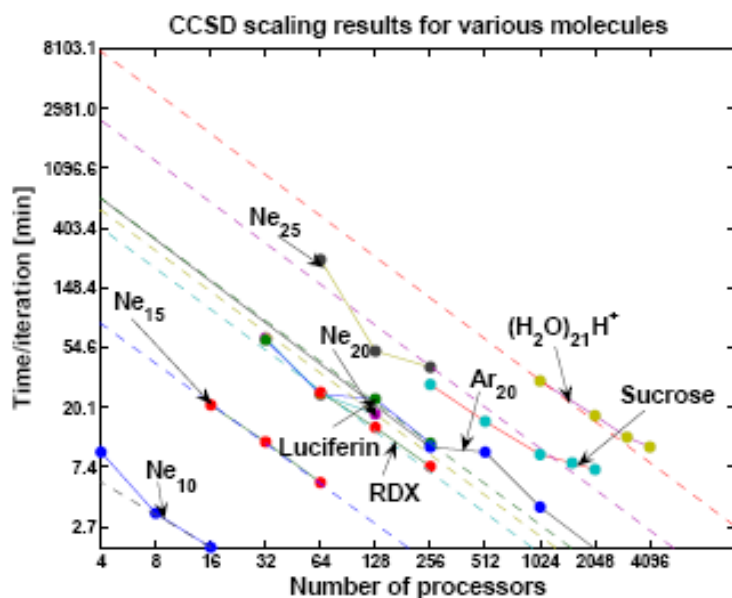
D. Further progress in the development of _ab initio dft_.

The idea of _ab initio dft_ is that the Kohn-Sham density functional one-electron structure can be built upon _ab initio_ correlated coupled-cluster and many-body perturbation theory methods, to correct the principal failing of dft methods; namely that they do not converge to the right answer in the basis set and correlation limit, unlike _ab initio_ wavefunction methods. On the other hand, wavefunction methods require a two-particle structure, which limits their application to large molecules, unlike DFT. Progress can be made by combining the best of both worlds. We have previously shown a number of results that conclusively prove the formal and numerical superiority of such an approach, but always at a cost in its implementation compared to conventional DFT. Papers **[4,5,13]** further contribute to this development.

Paper [**5**] addresses the issue of quasi-degeneracy in _ab initio dft_, using the Be isoelectronic sequence as an example. For this sequence, previous attempts by other authors to obtain the correct exchange and correlation potentials suffer from divergence. For our _ab initio dft_ approach, this does not happen because of the superior choice we make for our unperturbed hamiltonian, compared to the usual Kohn-Sham choice that is invariably used by DFT practioners. However, for the Be sequence, there is still a need to incorporate higher-order effects than is possible by using a MBPT(2) functional. Hence, we introduced a new coupled-cluster based

perturbation theory to add higher-order effects into what is still an attractive second-order approach. We call the new approach, CCPT2. With it we are able to show much better converged results for the Be sequence. This approach also has some advantages for other coupled-cluster problems, which we are pursuing.

Paper **[13]** asks the interesting question can we use a fraction of HF exchange to make the correlation potential that *ab initio dft* creates to be obtained more easily, and can we define an *exact one-particle theory* such that the orbital energies obtained from the one-particle Hamiltonian will provide virtually exact ionization potentials for **all** the occupied states of a molecule. We can indeed do that with the simple expedient of taking 50% HF exchange together with 50% OEP exchange, but it is necessary to also use our usual semi-canonical OEP-MBPT2 correlation potential to make this happen. This is a fascinating result as it means that numerically one can invent a one-particle, Hamiltonian that gives exact results. So this can be viewed as a frequency independent approximation to the Dyson operator or as a generalization of DFT that insists upon this IP property as an exact condition instead of the density that defines KS theory.

E.   Our intent in new work is to introduce an alternative, exact, correlated one-particle theory for electronic structure, for both its computational aspects and its conceptual ones. It will correctly describe self-interaction and charge-transfer, and dispersion. It also provides a systematic route toward exact solutions as more particles are added. We will also address the question of what quantities can we expect to be able to describe correctly within such a one-particle, correlated orbital theory (COT).That is, we insist that an $h^{eff}(1)$ be created such that

$$h^{eff}(1)\varphi_i(1)=\square_i\varphi_i(1), \quad \square_i=-I(i)$$

$$h^{eff}(1)\varphi_a(1)=\square_a\varphi_a(1), \quad \square_a=A(a)$$

In each case, the eigenvalues are the exact, principal ionization potentials, $I(i)$, and electron affinities, $A(a)$. The meaning of 'principal' means the energies required to remove an electron from any of the ith occupied orbitals, or to add an electron into any of the ath unoccupied orbitals. For the latter, many such energies will be negative, that is, will not correspond to bound anions and observed electron affinities. For I's, most of the principal ones will usually be seen experimentally except when a 'shake-up' has a very large intensity that masks the principal in that energy range. For our purposes, a shake-up in not a one-particle effect, so it falls outside the scope of our present exact COT. If we do an IP-EOM-CC calculation, matrix diagonalization will provide a set of n principal eigenvalues and vectors for n-electrons (orbitals). Similarly, EA-EOM-CC will provide the same A's for m-n unoccupied orbitals, where m is the dimension of the MO basis set. These, of course, will be exact in the limit of electron correlation and basis set. They are also equivalent to those obtained from effective one-particle theories as we can prove. Because h^{eff} is non-Hermitian, the

orbitals will compose both a right-hand and a left-hand set, with the same eigenvalues.

Hence, we first establish that an 'exact' one-particle theory of the type we propose exists. We achieve this by construction[25]. Furthermore, those equations can always be evaluated by doing coupled-cluster calculations. This is notably contrary to DFT, which is not based on 'constructive' proofs, but instead on existence proofs. Hence, there is seldom any independent way to assess the veracity of chosen approximations. But in our new theory an exciting prospect is that the equations can be used independently of doing the actual CC calculations, provided that an adequate approximation for the two-partcle interactions can be made, like that due to Colle and Salvetti, or for the two-particle density matrix in general as in density matrix functional theory. Unlike DFT, such an approach provides a litmus test for any two-particle approximation considered, since the eigenvalues of the associated potential have to reflect the exact properties we establish. Furthermore, in our constructive method, we can always make relevant coupled-cluster calculations to see what the right answers ought to be, and use this to immediately assess various approximations. We are currently making the initial computations to illustrate its use. Among other things, this theory will introduce a set of ionization(I) and electron attached (A) orbitals that associate with each orbital the exact principal I and A energies. So the difference between the HOMO and LUMO levels will be exactly the smallest I-A. In the case of solids this is the band gap, while for molecules, this theory should offer a new conceptual (and computational) basis for MO theory based upon exact I and A values.

Furthermore, I would also suggest that having this energy based scheme rather than a density based one (DFT) is vastly more suited to photo-electron spectra in general, a pervasive component of AFOSR' programs, such as in its applications to ionic liquids, and in the identification and classification of clusters via such PES experiments using anions, cations, and neutrals. The new theory I am proposing has to get I's and A's right, unlike DFT. And when needed, the corresponding CC applications can be made to keep the simplified theory, which is geared toward very large molecule applications, on target.

Archival publications during reporting period:

1.   R. J. Bartlett and M. Musial, "Coupled-cluster theory in quantum chemistry", Revs. of Modern Phys. **79,** 291-352 (2007).

2.   M. Musial, R.J. Bartlett, "Addition by Subtraction in Coupled Cluster Theory II. Equation-of-motion coupled cluster method for excited, ionized and electron-attached states based on the nCC ground state wavefunction", J. Chem. Phys. **127**, 024106/1-024106/9 (2007).

3. M.R. Berman, T. Tsuchiya, A. Gregusova, S.A. Perera and R.J. Bartlett, "HNNC radical and its role in the CH + N_2 reaction," J. Phys. Chem. A **111**, 6894-6899 (2007).

4. I. Grabowski, V. Lotrich and R.J. Bartlett, "*Ab initio* density functional theory applied to quasidegenerate problems," J. Chem. Phys. **127**, 154111/1-154111/10 (2007).

5. D. Bokhan and R.J. Bartlett, "Exact-exchange density functional theory for hyperpolarizabilities," J. Chem. Phys. **127**, 174102/1-174102/9 (2007).

6. A. Taube and R.J. Bartlett, "Improving upon CCSD(T):ΛCCSD(T). I. Potential energy surfaces," J. Chem. Phys. **128**, 044110/1-044110/13 (2008).

7. A. Taube and R.J. Bartlett, "Improving upon CCSD(T):ΛCCSD(T). II. Stationary formulation and derivatives," J. Chem. Phys. **128**, 044111/1-044111/9 (2008).

8. A. Taube and R.J. Bartlett, "Frozen natural orbital coupled-cluster theory: Forces and applications to decomposition of nitroethane," J. Chem. Phys. **128**, 164101/1 – 164101/17 (2008).

9. M. Musial and R.J. Bartlett, "Intermediate Hamiltonian Fock-space multireference coupled-cluster method with full triples for calculation of excitation energies," J. Chem. Phys. **129**, 044101/1-044101/10 (2008).

10. T.F. Hughes, N. Flocke and R.J. Bartlett, "Natural linear-scaled coupled-cluster theory with local transferable triple excitations: Applications to peptides," J. Phys. Chem. A **112**, 5994-6003 (2008).

11. T.F. Hughes and R.J. Bartlett, "Transferability in the natural linear-scaled coupled-cluster effective Hamiltonian approach: Applications to dynamic polarizabilities and dispersion coefficients," J. Chem. Phys. **129**, 054105/1 – 054105/13 (2008).

12. T. Kus and R.J. Bartlett, "Different equation-of-motion coupled cluster methods with different reference functions: The formyl radical," J. Chem. Phys. **129**, 104301/1 – 104301/11 (2008).

13. I.V. Schweigert and R.J. Bartlett, "Effect of the nonlocal exchange on the performance of the orbital-dependent correlation functionals from second-order perturbation theory," J. Chem. Phys. **129**, 124109/1 – 124109/8 (2008).

14. M. Musial and R.J. Bartlett, "Multireference Rock-space coupled-cluster and equation-of-motion coupled-cluster theories: The detailed interconnections," J. Chem. Phys. 129, 134105/1 – 134105/12 (2008).

15. V. Lotrich, N. Flocke, M. Ponton, A. Yau, A. Perera, E. Deumens and R.J. Bartlett, "Parallel implementations of electronic structure energy, gradient and Hessian calculations," J. Chem. Phys. 128, 194104/1-194104-15 (2008).

16. F. Cargnoni, T. Kus, M. Mella, and R. J. Bartlett, "Ground state potential energy surfaces and bound states of M-He dimers (M = Cu, Ag, Au). A theoretical investigation," J. Chem. Phys. **129**, 204307/1- 204307/12 (2008).

17. M. Musial and R.J. Bartlett, "Benchmark calculations of the Fock-space coupled cluster single, double, triple excitation method in the intermediate Hamiltonian formulation for electronic excitation energies," Chem. Phys. Letts. **457**, 267-270 (2008).

18. M. Musial and R.J. Bartlett, "Spin-free intermediate Hamiltonian Fock-space coupled-cluster theory with full inclusion of triple excitations for restricted Hartree Fock based triplet states," J. Chem. Phys. **129**, 244111/1-244111/6 (2008).

19. S.A. Perera, A. Gregusova, and R.J. Bartlett, "First calculations of $^{15}N - ^{15}N$ J values and new calculations of chemical shifts for high nitrogen systems; A comment on the long search for HN_5 and its pentazole anion," J. Phys. Chem. A, 10.021/jp809267y (2009).

20. T. Kus, V. Lotrich, and R.J. Bartlett, "Parallel implementation of the equation-of-motion coupled-cluster singles and doubles method and application for radical adducts of cytosine," J. Chem. Phys. **130**, 124122/1-124122/7 (2009).

21. A. Taube and R.J. Bartlett, "Rethinking linearized coupled-cluster theory," J. Chem. Phys. **130**, 144112/1 -144112/14 (2009).

22. T. Kus, V.F. Lotrich, A. Perera, and R. J. Bartlett, "An *ab initio* study of the $(H_2O)_{20}H^+$ and $(H_2O)_{21}H^+$ water clusters," J. Chem. Phys. **131**, 104313/1 – 104313/6 (2009).

23. T. Kus and R.J. Bartlett, "Improving upon the accuracy for doubly excited states within the coupled cluster singles and doubles theory," J. Chem. Phys. **131**, 124310/1 – 124310/10 (2009).

24. M. Musial, S.A. Kucharski, P. Zerzucha, T. Kus, and R.J. Bartlett, "Excited and ionized states of the ozone molecule with full triples coupled cluster methods," J. Chem. Phys. **131**, 194104/1 – 194104/10 (2009).

25. R. J. Bartlett, "Towards an exact correlated orbital theory for electrons," Invited Frontiers Article, Chem. Phys. Lett. **484**, 1-9 (2009)

In press:

R. J. Bartlett, M. Musial, V. Lotrich, T. Kus,"The Yearn to be Hermitian," in Recent Progress in Coupled Cluster Methods: Theory and Applications, Eds. Petr Carsky, Jiri Pittner, and Joe Paldus, Springer, 2010.

Publications submitted:

1. A. Melnichuk, A. Perera, and R.J. Bartlett, "Ab initio simulation of UV/Vis absorption spectra for atmospheric modeling: Method Design for bound and dissociative states of medium-sized molecules," submitted Phys. Chem. Chem. Phys. (2009).

2. A. Perera, A. Gregusova, and R.J. Bartlett, "The accuracy of computed ^{15}N nuclear magnetic resonance chemical shifts," submitted J. Theor. Anc Comp. Chem. (2009).

Special Invited Lectureships during reporting period:

June 2009 – Löwdin Lecture, Uppsala Universitet, Uppsala, Sweden

September 2008 – Eighth Triennial Congress of the World Association of Theoretical and Computational Chemistry (WATOC), Sydney, Australia upon receiving the Schrödinger Medal

December 2007 – "Coupled-Cluster Theory in Quantum Chemistry: The Emergence of a New Paradigm," THE BARTLETT LECTURE, 16th Conference on Current Trends in Computational Chemistry, Jackson, MS.

  (The honoree gives a lecture named for him/herself.)

July 2007 – CRANN Distinguished Lecturer, Trinity College, Dublin, Ireland

March 2007 – 3rd Annual Löwdin Lecture, University of Florida, Gainesville, FL

March 2007 – "Coupled-cluster Theory in Quantum Chemistry: The Emergence of a New Paradigm," AWARDS SYMPOSIUM, National ACS Meeting, Chicago, IL, upon receiving the ACS Award in Theoretical Chemistry

January 2007 – Coochbehar Professorship Lecture, Indian Association for the Cultivation of Science, Kolkata, India

Invited lectures at Professional Conferences during reporting period:

July 2009 – Canandian Conference on Computational Chemistry VII, Halifax, Nova Scotia

May 2009 – Air Force Office of Scientific Research Contractors Meeting, San Diego, CA

March 2009 – American Chemical Society Spring 2009 National Meeting, Salt Lake City, UT

March 2009 – Horiba International Conference on Simulations and Dynamics for Nanoscale and Biological Systems, University of Tokyo, Tokyo, Japan

December 2008 – Celebration of Forty Years of Theoretical Chemistry at Aarhus University, Aarhus, Denmark

September 2008 - Eighth Triennial Congress of the World Association of Theoretical and Computational Chemistry (WATOC), Sydney, Australia

July 2008 – Symposium on "50 Years of Coupled Cluster Theory," Institute of Nuclear Theory, University of Washington, Seattle, WA

July 2008 - Sixth Congress of the International Society for Theoretical Chemical Physics, Vancouver, Canada

June 2008 – "Ab initio DFT: The seamless connection with wave-function theory," UNEDF SciDAC Annual Workshop Pack Forest, WA

September 2007 – Local Correlation Methods: From Molecules to Crystals (LCC2007), Dresden, Germany

September 2007 – Symposium on Advanced Methods of Quantum Chemistry Physics, Toruń, Poland

May 2007- "Is there something better than ccsd(t) for molecular applications? Molecular Quantum Mechanics Analytic Gradients and Beyond, A meeting in honor of Peter Pulay, Budapest, Hungary

March 2007 **-** "Coupled-cluster theory: the emergence of a new paradigm" AWARDS SYMPOSIUM, National ACS Meeting, Chicago, IL

January 2007 – "Coupled-Cluster Theory for Large Molecules: The Natural Linear Scaled Coupled-Cluster Method," Recent Trends in Many-Body Methods for Electronic Structure and Properties of Atoms and Molecules, Bhubaneshwar (Orissa), India

January 2007 – "Natural Linear Scaling Coupled-Cluster Method and Some Other Advances for Large Calculations," NW Chem Meeting on Science Driven Petascale Computing and Capability Development at EMSL, Richland, WA

Invited Lectures at Universities and Laboratories

May 2009 – University of Colorado at Boulder, Boulder, CO

April 2009 – Texas Tech University, Lubbock, TX

January 2009 – Three lectures, Massey University, Albany, New Zealand

June 2007 – Univesité Louis Pasteur, Strasbourg, France

January 2007 – National Chemical Laboratory, Pune, India

Changes in research objectives, if any: None

Change in AFOSR program manager, if any: None

Extensions granted or milestones slipped, if any: Added Fourth Year to the project

Honors:

Received the 2009 Boys-Rahman prize of the Royal Society of Chemistry.

Received the 2008 Schroedinger Medal from the World Association of Theoretical or Computational Chemists (WATOC), Sydney, Australia

Symposium in honor of RJB, Corfu, Greece, ICCCMSE, 2008.

Symposium in honor of RJB, 235th American Chemical Society National Meeting, New Orleans, LA, April 2008

Honoree for the meeting, 16th Conference on Current Trends in Computational Chemistry, Jackson, MS. December, 2007.

Received the 2007 ACS Award in Theoretical Chemistry.

Coochbehar Professorship, Indian Association for the Cultivation of Science, Kolkata, India, 2007.